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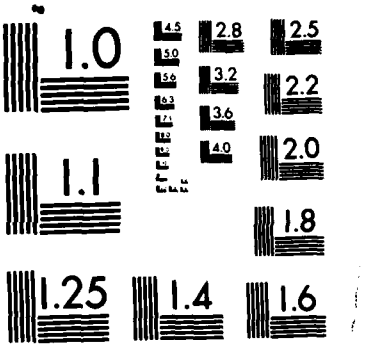

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Exact Dynamically Convergent Calculations of the Frequency-Dependent Density Response Function

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EXACT DYNAMICALLY CONVERGENT CALCULATIONS OF THE FREQUENCY-DEPENDENT DENSITY RESPONSE FUNCTION

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ABSTRACT

A general expression for the response function is derived by the method of recurrence relations. Memory effects appear as corrections to the dynamic RPA form. The dynamic structure for the 3d electron gas is calculated to third order and compared with Al data at a large wave vector. Also shown is the dynamic local-field term.

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The dynamic response in strongly interacting homogeneous many-fermion systems has drawn considerable attention recently.[1] Let such a many-body system be described by $H = H_o + V$, where H_o represents the kinetic energy and V the interaction energy, and the response in the system by the response function $\chi_k(\omega)$, where k and ω are, respectively, wave vector and frequency ($\hbar$=1). It is well known that the response function may be put in the form

$$\chi_k(\omega) = \chi_k^{(o)}(\omega) \,/(1 + \Lambda_k(\omega)\chi_k^{(o)}(\omega)) \qquad (1)$$

where $\chi_k(o)(\omega)$ is the response function due to H_o and $\Lambda_k(\omega)$ some unknown function of V. Various <u>dynamic</u> RPA theories are equivalent to taking $\Lambda_k(\omega)=\Lambda_k(0)\equiv\Lambda_k$.[2] For example, $\Lambda_k = v_k$ gives the <u>simple</u> RPA where v_k is the two-body interaction, and $\Lambda_k = v_k(1 - G_k)$ gives the <u>generalized</u> RPA where G_k is a local field term effective over the Thomas-Fermi length.[3,4] There are large numbers of RPA based studies and they have been routinely used to interpret experiments.[5]

The dynamic RPA's, however, can break down especially in the regime of metallic densities at large wave vectors. Clearly, one needs to restore the frequency dependence e.g., $\Lambda_k(\omega)= v_k\ (1 - G_k(\omega$ Several people have obtained asymptotic conditions for $G_k(\omega)$.[6-9] Otherwise, there are at present no exact general expressions known. For a 3d Coulomb gas Devreese et al[10] and Holas et al[11] have calculated $G_k(\omega)$ by some approximate techniques. Unfortunately, they find in their calculations several unphysical divergences. This sort of situation has limited our understanding of the dynamic structure of metals at large wave vectors. In particular, whether

the observed fine structure arises from multi-pair excitations or from some other strong correlations remain unresolved.[4] In this Letter, we obtain a general expression for $\Lambda_k(\omega)$ by the method of recurrence reltions[12] and perform exact dynamically-convergent calculations based on it. Our results are compared with Al data.

The time evolution of the density fluctuation operator ρ_k may be given an orthogonal expansion viz., $\rho_k(t) = \sum_{\nu=0}^{d-1} a_\nu(t)\, f_\nu$, where $\{f_\nu\}$ forms a complete set of basis vectors spanning the d-dimensional Hilbert space of ρ_k and a_ν's are autocorrelation functions. There exist recurrence relations RRI and RRII, respectively, for f_ν's and a_ν's:

$$f_{\nu+1} = \dot{f}_\nu + \Delta_\nu f_{\nu-1} \tag{2}$$

$$\Delta_{\nu+1}\, a_{\nu+1}(t) = -\dot{a}_\nu(t) + a_{\nu-1}(t) \tag{3}$$

where $0 \leq \nu \leq d-1$, $\dot{f}_\nu = i[H, f_\nu]$, $\dot{a}_\nu = da_\nu/dt$, $\Delta_\nu = (f_\nu, f_\nu)/(f_{\nu-1}, f_{\nu-1})$ where the inner product means the Kubo scalar product and by definition $f_{-1}=0$, $a_{-1} = 0$ and $\Delta_o = 1$. According to the method of recurrence relations, one obtains the basis vectors f_ν's by RRI (2) from which the recurrants Δ_ν's. One can then deduce the autocorrelation functions a_ν's by RRII (3) and obtain the time evolution of ρ_k.[13]

If we choose $f_o = \rho_k$, then by linear response theory $a_o(t) = (\rho_k(t), \rho_k)/(\rho_k, \rho_k)$, which is the relaxation function, and $\Delta_1 a_1(t) = \chi_k(t)/\chi_k$, where $\chi_k = (\rho_k, \rho_k)$. If $\nu=0$ in (3), we get

$$\Delta_1 a_1(t) = -\dot{a}_o(t). \tag{4a}$$

By applying the Laplace transform operator T and with $a_o(t=0) = 1$,

we obtain

$$\Delta_1 a_1(z) = 1 - z\, a_o(z) \quad . \tag{4b}$$

where $a_\nu(z) = T[a_\nu(t)]$. Hence, from (4b),

$$a_o(z) = (z + \Delta_1 b_1(z))^{-1} \tag{5}$$

where $b_1(z) = a_1(z)/a_o(z)$. Now combining (4b) and (5) and using the identity $\Delta_1 a_1(z) = \chi(z)/\chi$, suppressing k-dependence altogether, we get

$$\frac{\chi(z)}{\chi} = \frac{\Delta_1 b_1(z)}{z + \Delta_1 b_1(z)} \quad . \tag{6}$$

Since eq. (7) is valid for any Hermitian model, it also applies to H_o (ideal version). Now consider $\Delta_1 = (f_1, f_1)/(f_o, f_o)$. Since $f_1 = \dot{f}_o$ from (2), we have $f_1 = i[H, \rho_k] = i[H_o, \rho_k] = f_1^{(o)}$.[14] Hence,

$$\frac{\Delta_1^{(o)}}{\Delta_1} = \frac{\chi}{\chi^{(o)}} \quad . \tag{7}$$

We divide (6) by its ideal version and obtain

$$\frac{\chi(z)}{\chi^{(o)}(z)} = \frac{1}{\dfrac{b_1^{(o)}(z)}{b_1(z)} \left[\dfrac{z + \Delta_1 b_1(z)}{z + \Delta_1^{(o)} b_1^{(o)}(z)}\right]} \tag{8a}$$

$$\equiv \frac{1}{1 + \Lambda(z)\chi^{(o)}(z)} \quad . \tag{8b}$$

Observe that (8b) is in the form of (1). By using the ideal version of (6), we find from (8a,b) the desired expression:

$$\Lambda(z) = [(\chi)^{-1} - (\chi)^{(o)-1}] + \frac{z}{(f_1,f_1)}[(b_1(z))^{-1} - (b_1^{(o)}(z))^{-1}]$$

$$\equiv \Lambda + \lambda(z). \qquad (9)$$

The first bracketed term Λ is z-independent. Thus, the RPA theories are valid, i.e., $\Lambda(z) = \Lambda$, if and only if $b_1(z) = b_1^{(o)}(z)$.

We shall now examine the z-dependent part. Earlier, $b_1(z)$ was introduced in place of $a_1(z)/a_o(z)$. According to the method of recurrence relations[12] there is actually a whole family of $b_\nu(t) = T^{-1}[b_\nu(z)]$, $1 \leq \nu \leq d-1$, which define the time evolution of the generalized random force F_k for ρ_k as $F_k(t) = \sum_{\nu=0}^{d-1} b_\nu(t)\, f_\nu$. The random force lies in a linear manifold of the Hilbert space of ρ_k. The autocorrelation functions b_ν's, sometimes referred to as the memory functions, also satisfy a recurrence relation:

$$\Delta_{\nu+1} b_{\nu+1}(t) = -\dot{b}_\nu(t) + b_{\nu-1}(t) \qquad (10)$$

where $b_o(t) \equiv 0$ and $1 \leq \nu \leq d-1$. That is, for example,

$$b_1(t) = b_1(\Delta_2, \Delta_3, \ldots, \Delta_{d-1}; t) \quad . \qquad (11)$$

Hence, if $\Delta_\nu \neq \Delta_\nu^{(o)}$, $2 \leq \nu \leq d-1$, memory effects due to interaction are always present in the response function and are manifested through z dependence in $\Lambda(z)$.[15]

The recurrants Δ_ν's, which are relative norms of the basis vectors, are model-dependent. They are basic elements of the dynamic structure and their form shapes the time evolution. In

some special physical regimes of certain many-body models they can be calculated to any order and one can use them to obtain the memory function from RRII (10).[13] For noninteracting systems e.g., an ideal 3d electron gas, the recurrants are in effect known to all orders at T = 0 since $\chi_k^{(o)}(z=i\omega)$ is analytically given in the ground state. But for interacting systems generally, only the first few orders of the recurrants have been accurately calculated presently. Hence, one cannot obtain their memory function by (10) and one cannot use the general expression (9) to explicitly calculate e.g., Im $\chi_k(\omega)$ for metal densities at large wave vectors. We propose here a technique by which one can use (9) to calculate $\Lambda(z)$ term-by-term up to the available order of the recurrants given that the "ideal" recurrants are known to all orders.

From (9) and (11) we see that

$$\lambda = \lambda\left(\{\Delta_\nu\}; \{\Delta_\nu^{(o)}\}; z\right), \quad \nu \geq 2 \tag{12}$$

assuming $d = \infty$. Hence we can write

$$\lambda = \lim_{n \to \infty} \lambda_n \tag{13}$$

where

$$\lambda_n = \lambda(\Delta_2 \ldots \Delta_n \; \Delta_{n+1}^{(o)} \ldots \Delta_\infty^{(o)}; \{\Delta_\nu^{(o)}\}; z) \; . \tag{14}$$

The process of replacing λ by λ_n has the following significance: If λ_n is used in place of λ in (9), the resulting $\chi(z)$ satisfies the frequency moment sum rules exactly up to and including the 2n+1 st. It satisfies the higher moments to the accuracy of the substitution of Δ_m by $\Delta_m^{(o)}$, $m \geq n+1$.[16]

By this process one can obtain an expression for the response function in terms of the recurrants which is exact to a given order. One can continue this process to the highest available recurrant. An infinite-order expression evidently is equivalent to an exact expression for the response function.

Using (9) and RRII, we can systematically obtain λ_n e.g.

$$\lambda_1 = 0 \tag{15}$$

$$\chi^{(o)}\lambda_2 = \eta_2 Q(z)$$

$$\chi^{(o)}\lambda_3 = (\eta_2 - \eta_3 R(z))Q(z)/(1 + \eta_3 R(z))$$

etc. where $\eta_j = \Delta_j/\Delta_j^{(o)} - 1$, $j = 2,3$

$$Q(z) = \chi^{(o)}/\chi^{(o)}(z) - z^2/\Delta_1^{(o)} - 1$$

$$R(z) = 1 - \gamma Q(z), \quad \gamma = \Delta_1^{(o)}/\Delta_2^{(o)} .$$

Observe that $\lambda \to \lambda_1$ gives the generalized RPA. For $k \simeq k_F$, where k_F is the Fermi vector, multipair excitations exist which are contained in $\Delta_2\Delta_3$ etc. They can, therefore, contribute to the response function via frequency dependence beyond first order. The convergence of our term-by-term calculations should be relatively rapid since our procedure uses infinite continued fractions at all stages which are known to give good convergence.[17] Finite order calculations are meaningful if $\chi^{(o)}(z) \neq 0$.

To illustrate our technique, we calculate the dynamic structure factor $S_k(\omega) = -\pi^{-1}$ Im $\chi(z=i\omega)$ for the 3d electron gas to third order, the highest order possible based on the presently available recurrants which are $\Delta_1\Delta_2\Delta_3$. For our calculations we

set $k = 1.6\ k_F$ and $r_s = 2.0$ (cf. Al $r_s = 2.07$). For these values we find: $\eta_2 = 0.1297$, $\eta_3 = 0.0364$, and $\gamma = 0.5619$.

Shown in Fig. 1A is the first-order corresponding to the generalized RPA (dotted line). It shows almost no fine structure. The second order (dash-dot line) and the third-order (solid line) begin to show some structure. The calculated amplitudes are all absolute. Observe that in our finite order calculations $S_k(\omega)=0$ for $\omega \geq 5.76\ \varepsilon_F$.[18] In Fig. 1B the third-order dynamic structure (solid line) is compared with the simple RPA (dotted line) and Al data (dashed line).[19] The experimental amplitude is adjusted to coincide with our third-order calculated one. The simple RPA-calculated amplitude is absolute. We observe that the third-order calculated structure factor shows some resemblance to the experimental curve especially in the shoulder. The peak position is much closer to the experimental peak position than that of the simple RPA.[20]

Using the definition $\underline{\underline{\lambda}}_k(\omega) = v_k(1-G_k(\omega))$ one can also extract the corresponding frequency-dependent local field term $G_k(\omega)$. These results are shown in Fig. 2. The first-order (dotted line) is absent in Im $G_k(\omega)$ since $\lambda_1 = 0$. The second-order (dash-dot lines) and third order (solid lines) are well-behaved, containing no infinities. In Re $G_k(\omega)$ there are cusp-like peaks at $\omega \approx 0.64\ \varepsilon_F$ and $5.76\ \varepsilon_F$. It is interesting to note that Devreese et al[10], Holas et al encountered divergences in their calculation of $G_k(\omega)$ at approximately these frequencies.

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13. For applications see M. H. Lee, Phys. Rev. Lett. 51, 1227 (1983); Lee et al ibid 52, 1579 (1984), Phys. Rev. A29, 1561 (1984); M. H. Lee & J. Hong ibid B30, 6725 (1984); J. Florencio & M. H. Lee ibid A31, 3237 (1985).
14. We note that $[V, \rho_k] = 0$ for $V = \frac{1}{2}\sum v_k \rho_k \rho_{-k}$. This result holds for Bose particles and our work applies to Bose systems. For Use of dynamic RPA's to Bose systems, see S. W. Lovesey

Also see P. Grigolini et al, Phys. Rev. B27, 7342 (1983) & M. Giodano et al, Phys. Rev. A28, 2474 (1983).

et al Phys. Rev. Lett. 33, 1356 (1975). To obtain eq. (7), we use the well-known relation $(\dot{\rho}_k, \dot{\rho}_k) = \rho_o \, k^2/Z_m$, where ρ_o is the number density.

15. For the 2d electron gas at long wavelenghts M. H. Lee & J. Hong [Phys. Rev. Lett. 48, 6349 (1982)] showed that $\Delta_1 \neq \Delta_1^{(o)}$, but $\Delta_\nu = \Delta_\nu^{(o)}$, $\nu \geq 2$. This accounts for the RPA work of A. Holas et al, Phys. Rev. B27, 598 (1983).

16. The frequency moment sum rules are $\langle\omega^{2n+1}\rangle = -\int_{-\infty}^{\infty} d\omega \, \omega^{2n+1} \frac{\text{Im } \chi(\omega)}{\pi \chi}$, $n = 0,1,$ These moments are expressible in terms of the recurrants e.g. $\langle\omega\rangle = \Delta_1$, $\langle\omega^3\rangle = \Delta_1(\Delta_1 + \Delta_2)$, $\langle\omega^5\rangle = \Delta_1((\Delta_1 + \Delta_2)^2 + \Delta_2 \, \Delta_3)$, etc. The process $\lambda \to \lambda_1$ means: $\langle\omega\rangle = \Delta_1$, $\langle\omega^3\rangle = \Delta_1(\Delta_1 + \Delta_2^{(o)})$, etc. Hence, the first moment (f sum rule) is exact, but the third and higher moments are not exact because of the substitution of Δ_2 by $\Delta_2^{(o)}$, Δ_3 by $\Delta_3^{(o)}$, etc. If $\lambda \to \lambda_5$, the first, third and fifth moments are exact. The seventh and higher moments are approximate by the replacement of Δ_4 by $\Delta_4^{(o)}$, Δ_5 by $\Delta_5^{(o)}$ etc.

17. $\chi(z)$ is an infinite continued fraction of z (see Ref. 12). Continued fractions are known to yield improved convergence. See e.g. W. B. Jones and W. J. Thron, Continued fractions (Addison-Wesley, Reading 1980).

18. In finite order calculations $S_k(\omega) = 0$ if $\text{Im } \chi_k^{(o)}(\omega) = 0$. To obtaim the high frequency tail (see Fig. 1B) one must consider an infinite order calculation.

19. P. M. Platzman & P. Eisenberger, Phys. Rev. Lett. 33, 152 (1974).

20. There is a controversy on the difference of approximately $2\varepsilon_F$ between the experimental peak positions and the simple RPA-based calculated positions. See F. Green et al Phys. Rev. Lett. 48, 638 (1982) & Phys. Rev. B31, 2796 (1985).

Figure Captions

1. Dynamic structure vs frequency. A. first-order (dotted), second-order (dash-dot), third-order (solid). B. experimental (dash), simple RPA (dotted), third-order (solid). ε_F Fermi energy.

2. Dynamic local field correction vs frequency. First-order (dotted), second-order (dash-dot), third-order (solid). ε_F Fermi energy.

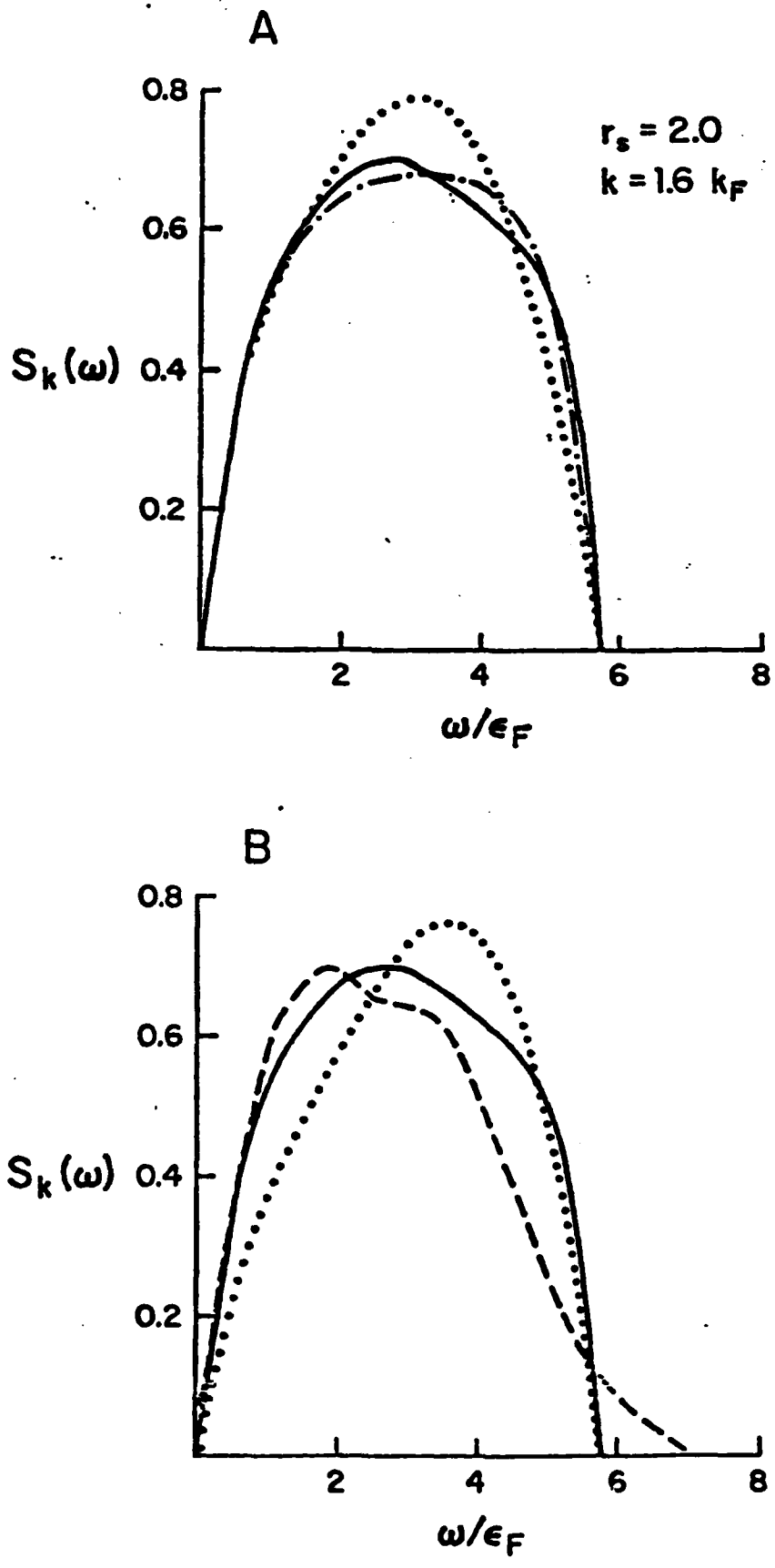
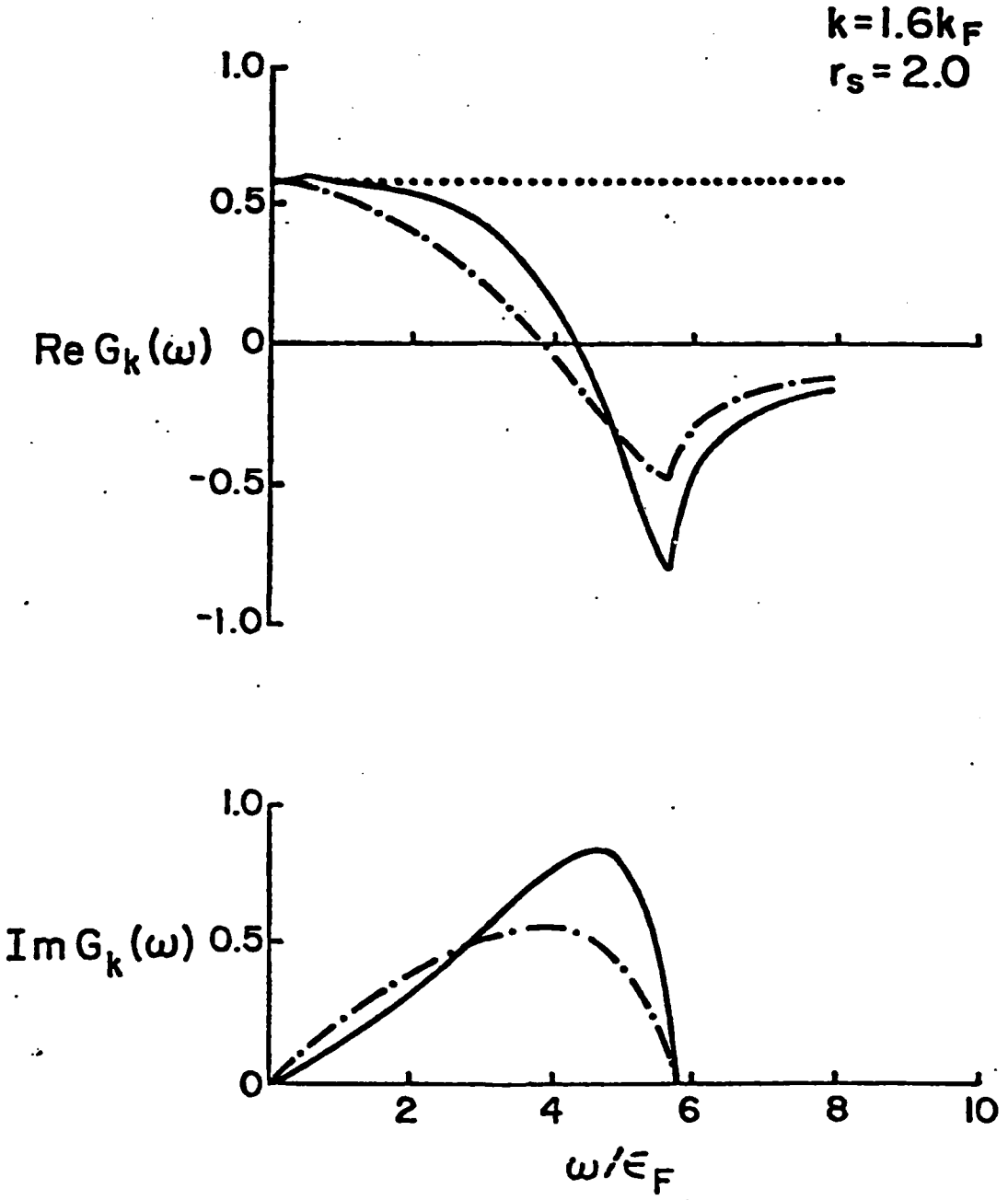

A
0.8
0.6
0.4
0.2
$S_k(\omega)$
$r_s = 2.0$
$k = 1.6\ k_F$
2
4
6
8
ω/ϵ_F
B
0.8
0.6
0.4
0.2
$S_k(\omega)$
2
4
6
8
ω/ϵ_F

Fig. 2



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